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Stable corrugated state of the two-dimensional electron gas.

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Abstract. A corrugated and stable ground state is found for the two dimensional electron gas at intermediate densities, $r_s \approx 25$. This state is obtained with a self consistent Hartree–Fock method with modulated trial wave functions in the deformable jellium model. The state is shown to appear for paramagnetic and ferromagnetic systems. The electron gas is shown to be non–corrugated for high metalic densities. The transition to the corrugated state occurs at $r_s \approx 4.8$ in the paramagnetic and $r_s \approx 6.8$ in the ferromagnetic cases which is much lower than the corresponding 3D case. The overall stability against magnetic transitions is studied.

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The electron gas is a cornerstone of the many-body quantum theory applications to solid state physics [1]. Much effort has been devoted recently to the study of this system in the two dimensional (2D) case. Important applications have lead these studies. First, the realization that the electronic motion in the new high-temperature superconducting materials occurs mostly in planes has encouraged the development of 2D electron gas models in order to explain the high-temperature superconductivity [2]. Second, when an external magnetic field is present the two dimensional system develops new interesting properties such as the fractional statistics and the quantum Hall effect [3]. The study of the quantum Hall effect has motivated many calculations of the energy spectrum of two dimensional electron systems in the presence of magnetic fields applied perpendicularly to the electronic layer [4, 5]. The 2D electron gas has been also used as a model for metal-oxide-semiconductor (MOS) structures, heterostructures and superlattices [6, 7]. The transport properties of the 2D electron gas are also a matter of great interest in semiconductor physics [8].

Many of the techniques developed for the three dimensional (3D) system have already been applied to the 2D electron gas. For instance, the succesfull density functional theory [9, 10] has been also applied to the 2D electron gas in a transverse magnetic field [11]. Ground state properties of the 2D electron gas have been obtained using a variational correlated-basis-function (CBF) approach [12], the ladder approximation [13] and the effective-potential expansion method [14]. More recently, the ground state properties of this system in the jellium model have been studied using more accurate variational Monte-Carlo and the Green's-function Monte-Carlo methods [15]. However this exact solutions are in practice restricted to a few hundred particles [16], as is the case with the stochastic simulations of the Schrodinger

equation [17].

A time honored approach that we have exploited for the study of the 3D electron gas is the Hartree-Fock (HF) method. Our approach has been to obtain self-consistency for a set of modulating functions combined with the deformable jellium hypothesis [18]. This is a very powerful non-perturbative technique that allows a direct evaluation of ground state properties in the strong coupling region of low densities such as is the case of the transition to the Wigner crystal. In this work, this method is applied to evaluate ground state properties of the 2D electron gas.

One of the peculiarities of the electron gas is that in the low density regime the potential energy becomes relatively more important than the kinetic and it is expected that the electronic density becomes nonuniform in order to minimize the energy. Therefore at low densities, the particles will form a periodic crystalline array, this was first proposed by Wigner [19]. The HF method with the modulating set of basis functions has the built-in capability of describing both the metalic region and the low density region in a unified non-perturbative fashion. As in the 3D system, the self-consistent HF solution for the 2D electron gas at metallic densities is the plane wave (PW).

However, a recurrent problem in the study of the low density transition to the Wigner crystal is the instability of the electron gas with respect to density variations. The usual way out of this problem is to postulate that the background compensates this instability. This hypothesis is difficult to apply in the deformable jellium model because the static part of the background energy is already incorporated into the model. One might always argue that some unknown dynamical effect could solve the problem, but this approch merely postpones the difficulty. It would be logically much

better if the electron system in the corrugated phase would exhibit a stable behavior.

In the past, some indication of such a stable HF ground state has been reported by us for the 3D electron gas [20]. However this was considered only a preliminary result because the convergence of the calculation was not good enough in this system at low densities. Because the growth of the required computational resources dramatically decreases in going from three to two dimensions one might expect to obtain a more reliable result in the 2D electron gas.

Consider the system of N electrons, interacting via a Coulomb potential $V(r_{ij}) = e^2/r_{ij}$, where $r_{ij} = |r_i - r_j|$, immersed in a positive background in an area A. If the thermodynamical limit is considered, then $N \longrightarrow \infty$, $A \longrightarrow \infty$ with $\sigma = N/A$ constant. Schematically, the HF Hamiltonian equation of this system has the terms

$$H = T_e + V_{bb} + V_{be} + V_D + V_{EX}, \tag{1}$$

where the subindices e and b refer to electron and background respectively, and V_D and V_{EX} are the direct and exchange terms of the electron-electron interaction, the potential V is the Coulomb interaction and T_e is the electronic kinetic energy. Atomic units are used throught this work.

In the deformable jellium model, the neutralizing background is requiered to deform to provide local neutrality. One consequence of this hypothesis is to diminish the energy of the system. The condition that defines the deformable jellium is [21]

$$< V_D > + < V_{bb} > + < V_{be} >= 0, \tag{2}$$

i.e. the terms of the background energy are identically canceled with the direct term

of the particle-particle interaction.

The trial state functions in the Slater determinant are taken to be the usual PW's multiplied by modulating functions. As usual [18], the minimal modulating frecuency, q_0, is obtained via de orthonormality condition of the orbitals. The orbitals proposed are of the form

$$\varphi_k(r) = \frac{e^{ik\cdot r}}{\sqrt{A}} \sum_{n_x,n_y=0}^{\mathcal{N}} C_{n_x n_y} \cos(q_0 n_x x) \cos(q_0 n_y y), \tag{3}$$

where A is the area in which periodic boundary conditions are imposed. The coefficients C_{n_x,n_y} are assumed to be independent of k. These coefficients are self-consistently determined by the HF equations with the orthonormality condition included. The first term in this expansion $n_x = n_y = 0$ is the PW solution. For the upper limits in the sums we select $\mathcal{N}_x = \mathcal{N}_y = \mathcal{N}$; in that way, when the solution is different from the PW, the system has a periodic density centered on a square lattice. The number of terms in the expansion is given by $(\mathcal{N}+1)^2$. Other lattices can be obtained by the usual modification of the Brillouin zone geometry.

The energies for the normal paramagnetic and the ferromagnetic states are evaluated in order to determine the magnetic nature of the ground state. In the paramagnetic case, each orbital within the Fermi sphere of radius k_F has double occupancy. While in the ferromagnetic case, the orbitals within a sphere of radius $\sqrt{2}k_F$ are singly occupied.

The ground state energy per particle with the orbitals of Eq.(3), requires the evaluation of terms of the form

$$\frac{T}{N} = \frac{1}{r_s^2}\sum_{\boldsymbol{n}} |C_{\boldsymbol{n}}|^2(1+8n^2), \tag{4}$$

$$\frac{V}{N} = -\frac{\sqrt{2}/(32\pi^2)}{r_s}\sum_{\boldsymbol{n_1}}\sum_{\boldsymbol{n_2}}\sum_{\boldsymbol{n_3}}\sum_{\boldsymbol{n_4}} C_{\boldsymbol{n_1}}{}^* C_{\boldsymbol{n_2}}{}^* C_{\boldsymbol{n_3}} C_{\boldsymbol{n_4}} I(\boldsymbol{n_1},\boldsymbol{n_4}) F(\boldsymbol{n_1},\boldsymbol{n_2},\boldsymbol{n_3},\boldsymbol{n_4}), \tag{5}$$

where r_s is the density parameter, in Bohr radius and N is the number of particles. $\boldsymbol{n}$ is a two dimensional vector $\boldsymbol{n} = n_x\boldsymbol{i} + n_y\boldsymbol{j}$. The function $I(\boldsymbol{n_1},\boldsymbol{n_4})$ that stems from the integrals of the Coulomb potential in terms of the components of $\mathbf{n_1}$ and $\mathbf{n_4}$ has been numerically evaluated. Finally $F(\boldsymbol{n_1},\boldsymbol{n_2},\boldsymbol{n_3},\boldsymbol{n_4})$ is a sum of 64 terms which are products of Kronecker δ functions in the components of the four n_i's. Some simplification can be obtained in the exchange term where 4^4 terms reduce to 4^3 because of symmetry considerations. Calculations for each value of the density parameter r_s can be carried out. The region of densities reported in this work is $3 < r_s < 100$.

Calculations were carried out to determine the coefficients $C_{\mathbf{n}}$ self-consistently, with an approximation of 10^{-5} with respect to the last iteration. The value of the upper limit in the sums was changed from $\mathcal{N} = 1$ up to 12, in order to obtain results for the ground state energy independent of $\mathcal{N}$. We get convergence for the energy results in a wide interval of r_s, with a function with up to 169 terms. The evaluation of the energy results for ten points with the $\mathcal{N} = 12$ expansion required about 150 VAX-780 equivalent hours.

The self-consistent solution both for the paramagnetic and ferromagnetic states, was the PW in the high density region. The value of r_s where the electronic density changes from constant to periodic defines the transition point to the charge density

waves (CDW), which at lower densities goes to the Wigner crystal [18]. Near the transition point the periodic density is not very pronounced, but at lower densities it becomes increasingly sharper.

The difference in the ground state energy per particle between the PW case and the self-consistent solution, in terms of the density parameter, is shown in Fig. 1. We display the results for the paramagnetic and ferromagnetic systems in Figs. 1a and 1b, respectively. In the graphics, the curves for different values of $\mathcal{N}$ are drawn. The transition from PW to a modulated solution appears at a greater density in the paramagnetic than in the ferromagnetic system. For $\mathcal{N} = 1$ and 2 the transition point to the periodic density depends in the number of terms in the state function. Beginning with $\mathcal{N} = 3$, this transition always occurs at $r_s = 4.8$ in the normal system, and at $r_s = 6.8$ for the completely polarized case. The value obtained for the transition point, $r_s = 4.8$, in the 2D paramagnetic system is lower than the result we have previously obtained in the corresponding 3D electron gas of $r_s = 26$ [20]. The values for the transition to the CDW Wigner-type crystal in this work are below the results reported in Ref. [10] with the density functional method for the 2D electron gas. This is also different from the 3D case where the two models predict a similar transition value for r_s. The transition values in this work are also significatively lower than the value of $r_s = 40$ obtained for the non-corrugating background of the usual jellium model [15], and are closer to the metalic densities.

It follows from Figs. 1a and 1b that a satisfactory convergence in the energy is obtained in the paramagnetic system in the intermediate density region, up to $r_s \approx 28$. A reasonable convergence is obtained at densities up to $r_s \approx 50$ for the ferromagnetic energy. We have to go to greater values of $\mathcal{N}$ if we were to look for a

greater degree of convergence in the energy results at lower densities.

In Table 1 we show the ground state energy per particle for the normal system in order to observe the convergence of the energies at the densities considered. We present nine different values of the upper limit in the sums, and four different densities. The ferromagnetic case displays a qualitatively similar behavior.

In Figs. 2a and 2b the ground state energy per particle is plotted for the two systems. The results are shown for the PW and for different values of $\mathcal{N}$. Immediately after the transition to periodic electronic density, we can observe in the energy curves a region where the slope changes. Then the curves with $\mathcal{N} = 12$ show a minimun at $r_s = 20$ in the normal system, and at $r_s = 30$ for the fully-polarized case. That means that there is a region of positive pressure, as it also occurs in the metallic density region (where the HF solution is the PW). This is a new behavior from those obtained so far for the energy dependence on the density. A similar result was obtained for the 3D case [20]. However the poor convergence of the calculation for the 3D system at values greater than $r_s = 50$ makes the 3D result preliminary.

In order to get an idea of how the results reported here compare with those obtained with different models and methods of calculation, we also include in Fig. 2 the results reported for the GFMC [15] for the 2D jellium. We observe that the 2D electron gas in the deformable jellium is a more stable system than the gas in the jellium, at intermediate and high densities ($r_s \geq 10$).

Let us finally study the stability of the 2D deformable jellium against magnetic transitions. In Fig. 3 the energies in the paramagnetic and ferromagnetic cases, obtained with the state function of Eq. (3) with $\mathcal{N} = 12$, are compared. The ground

state of the 2D electron gas in the deformable jellium calculation is a corrugated paramagnetic from $r_s = 6.5$ up until $r_s = 24$. After this point the ground state turns to be a corrugated ferromagnetic one. Not shown in the graphic is the region below $r_s = 5$ where starting with $r_s \approx 2$ up to 6.5, the ferromagnetic PW is the HF ground state.

In conclusion, the deformable jellium model confirms that the usual uniform PW solution in a ferromagnetic configuration is the HF ground state of the 2D electron gas for densities between $r_s \approx 2$ up to $r_s \approx 6.5$. At this point the system is predicted to have a transition to a paramagnetic corrugate state. Then at lower densities $r_s \approx 24$ the electron gas will show a magnetic transition to a ferromagnetic configuration. More remarkably, two metastable states are predicted by this model, one paramagnetic at $r_s \approx 20$ and the second at $r_s \approx 30$, in a ferromagnetic configuration. One might wonder what the effect of the non-spin correlations would be. A partial answer can be obtained at least for static correlations by introducing a screened Coulomb interaction. In the past we have computed the effect of a screened Coulomb interaction on the energy spectrum and the ground state energy of the 3D electron gas [18, 22]. The only effect that one expects from this type of correlations is to move the transition point to CDW to a lower density and as the range of the interaction is diminished, to move the energy of the system up. Therefore the qualitative behavior of the metastable states is not expected to change.

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References

[1] D. Pines, *The Many-Body Problem*, (W.A. Benjamin, Reading Mass., 1962).

[2] Y. Takada, *Phys. Rev. B* **39,** 11575 (1989).

[3] R. B. Laughlin, *Ann. Phys.* **191**, 163 (1989).

[4] M. P. Chaubey and C. M. Van Vliet, *Phys. Rev. B* **34,** 3932 (1986).

[5] R. B. Laughlin, *Phys. Rev B* **23,** 5632 (1981).

[6] *Two-dimensional Systems, Heterostructures and Superlattices,* edited by G. Bauer, F. Kuchar and H. Heinreich (Springer,Berlin,1984);

[7] J. M. Lagemaat, G. E. W. Bauer, J. J. Harris and C. T. Foxon, *Phys. Rev. B* **38,** 439 (1988).

[8] A. Gold, *Phys. Rev. B* **35,** 723 (1987).

[9] G. Senatore and G. Pastore, *Phys. Rev. Lett.* **64,** 303 (1990); M. P. Das and J. Mahanty, *Phys. Rev. B* **38,** 5713 (1988).

[10] L. M. Sander, J. H. Rose and H. B. Shore, *Phys. Rev. B* **21,** 2739 (1980).

[11] Swapan K. Ghosh and Asish K. Dhara, *Phys. Rev. A* **40,** 6103 (1989).

[12] Hock-Kee Sim, R. Tao and F. Y. Wu, *Phys. Rev. B* **34,** 7123 (1986).

[13] S. Nagano, K. S. Singwi and S. Ohnishi, *Phys. Rev. B* **29,** 1209 (1984); D. L. Freeman, *J. Phys. C* **16,** 711 (1983).

[14] Y. Takada, *Phys. Rev. B* **30,** 3882 (1984).

[15] B. Tanatar and D. M. Ceperley, *Phys. Rev. B* **39,** 5005 (1989).

[16] D. Ceperley, *Phys. Rev. B* **18,** 3126 (1978).

[17] D. M. Ceperley and B. J. Alder, *Phys. Rev. Lett.* **45,** 566 (1980).

[18] M. A. Ortíz and R. M. Méndez-Moreno, *Phys. Rev. A* **36,** 888 (1987).

[19] E. P. Wigner, *Trans. Faraday Soc.* **34,** 678 (1938).

[20] R. M. Méndez-Moreno, M. A. Ortíz and M. Moreno, *Phys. Rev. A* **40,** 2211 (1989).

[21] S. Orozco, M. A. Ortíz and R. M. Méndez-Moreno, *Phys. Rev. A* **41,** 5473 (1990).

[22] R. M. Méndez-Moreno and M. Moreno, *Phys. Rev. A* **41,** 6662 (1990).

Figure Captions

Fig. 1: Energy difference per particle, in Rydbergs, between the trivial PW and the HF expansion of Eq. (3), as a function of the parameter r_s, in Bohr radius. The results are given for different values of $\mathcal{N}$. The various curves are labeled by the corresponding $\mathcal{N}$ value . Two sets of curves are given: (a) paramagnetic system, (b) ferromagnetic system.

Fig. 2: Energy per particle, in Rydbergs, as a function of r_s: (a) the paramagnetic system and (b) the ferromagnetic one. The different curves are labeled by the value of the corresponding $\mathcal{N}$. The crosses are the values given in Ref. [15].

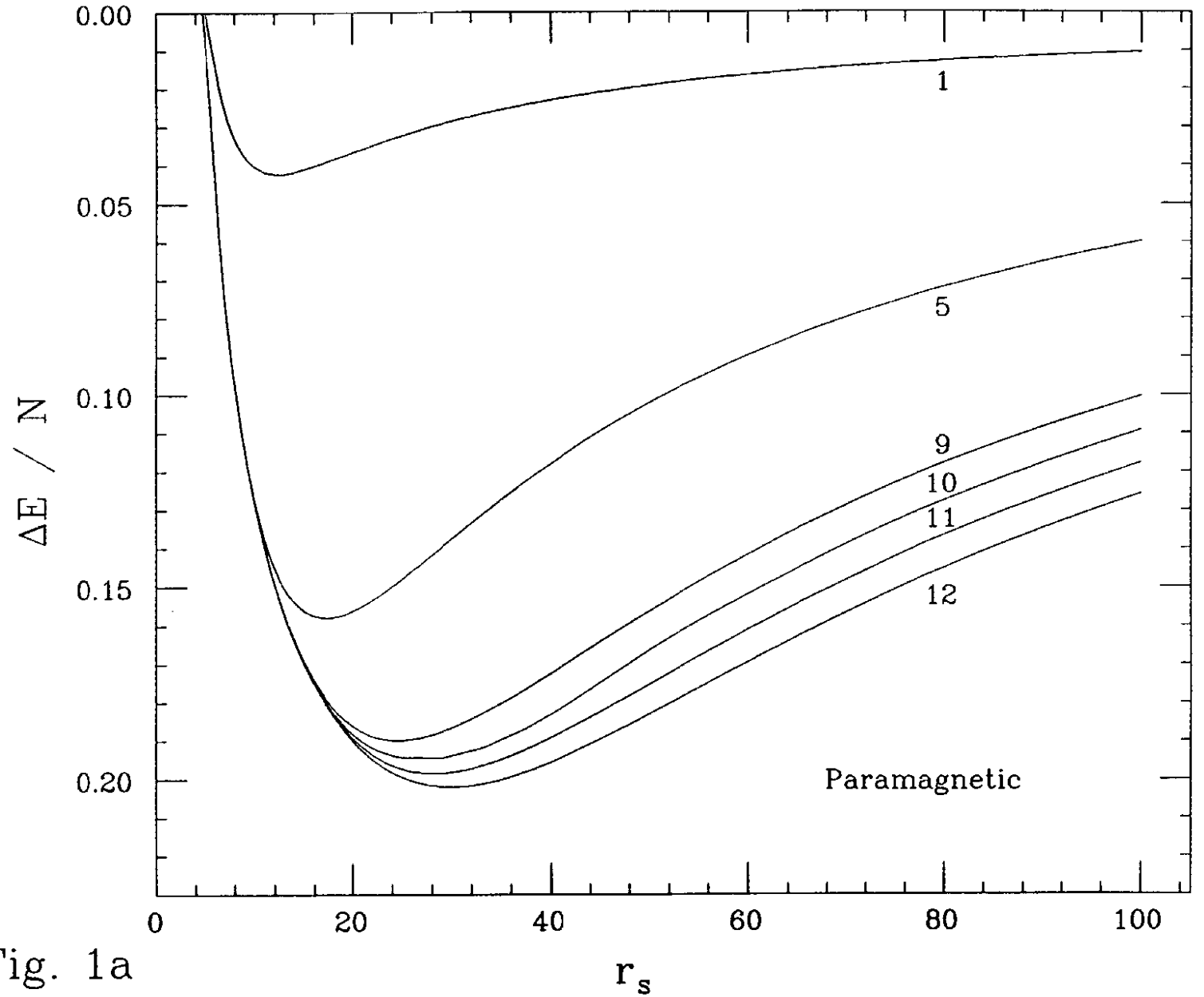
Fig. 3: Ground state energy per particle,in Rydbergs, of the 2D electron gas in terms of the parameter r_s. The full line corresponds to the ferromagnetic phase and the dashed line to the paramagnetic one.

Table Captions

Table 1: Ground state energy per particle of the paramagnetic system as a function of the number of terms in the state-function. The results are given at four different densities that involve the intermediate and high density region.

Table 1.

$\mathcal{N}$	$r_s = 10$	$r_s = 20$	$r_s = 30$	$r_s = 40$
0	-0.1100	-0.0575	-0.0389	-0.0294
1	-0.1503	-0.0941	-0.0674	-0.0524
3	-0.2222	-0.1706	-0.1312	-0.1057
5	-0.2376	-0.2137	-0.1764	-0.1474
7	-0.2381	-0.2345	-0.2063	-0.1786
9	-0.2381	-0.2436	-0.2256	-0.2019
10	-0.2381	-0.2457	-0.2321	-0.2111
11	-0.2381	-0.2469	-0.2371	-0.2186
12	-0.2381	-0.2475	-0.2409	-0.2250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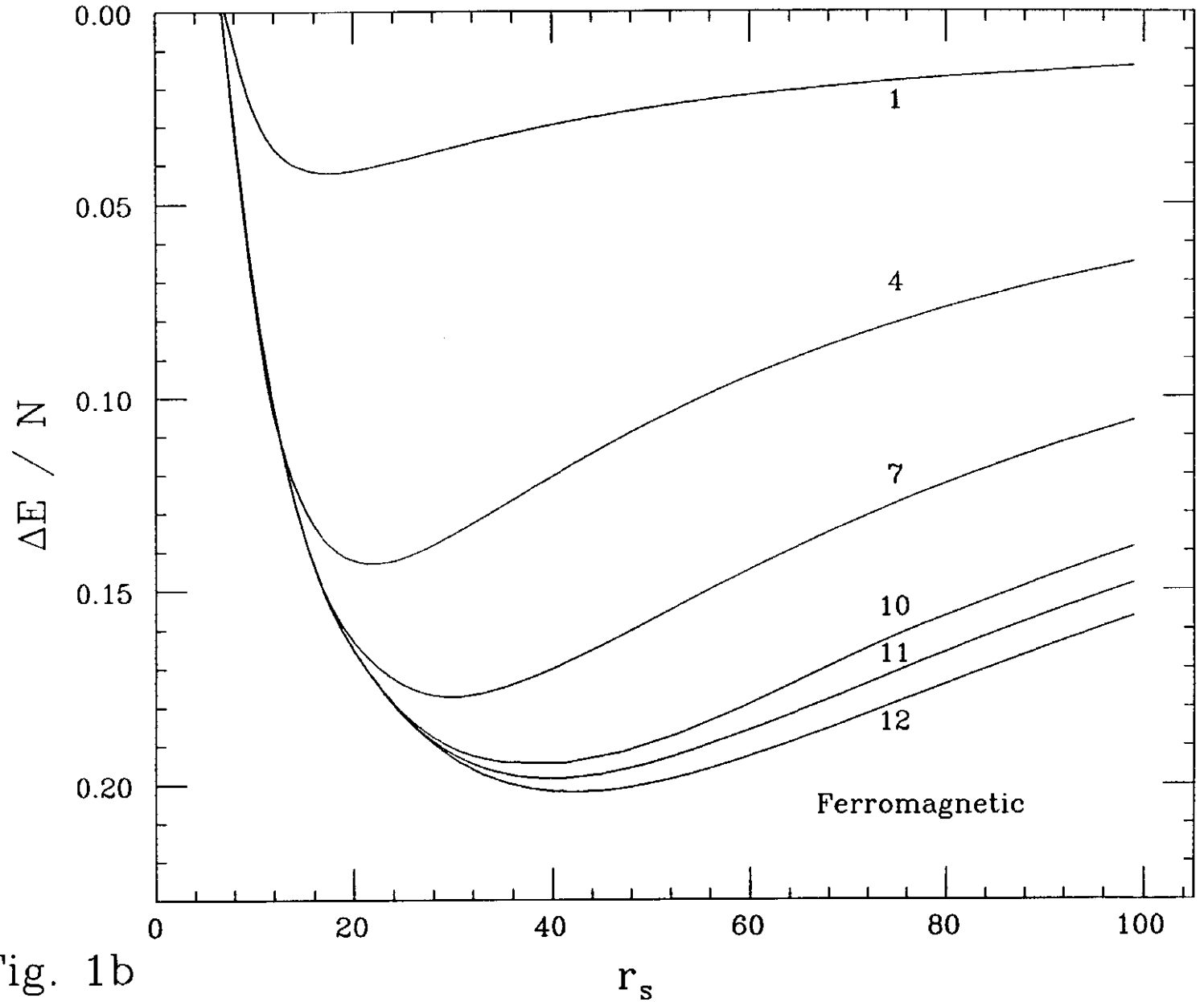
12
Paramagnetic

Fig. 1a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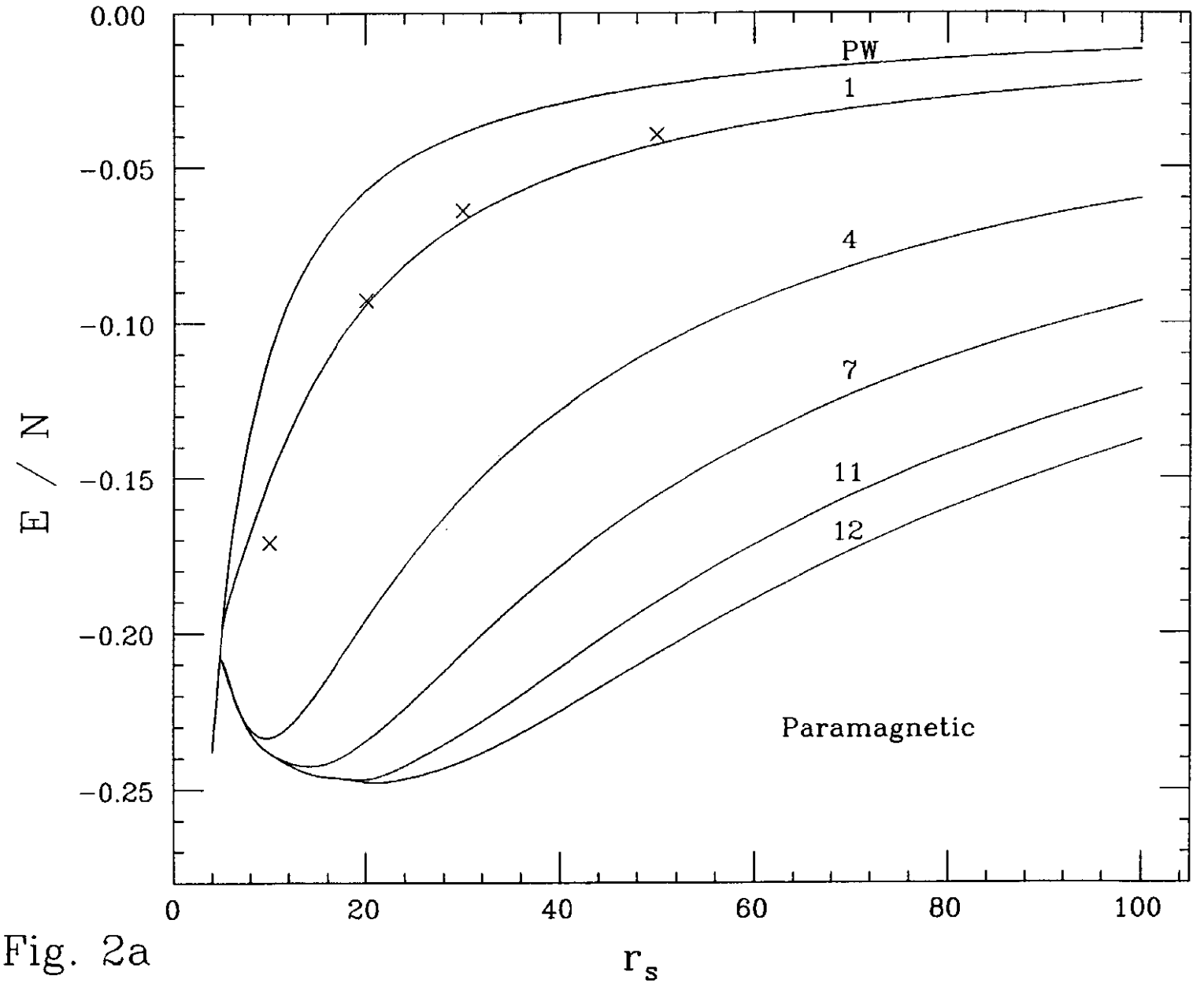
Ferromagnetic

Fig. 1b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Paramagnetic

Fig. 2a

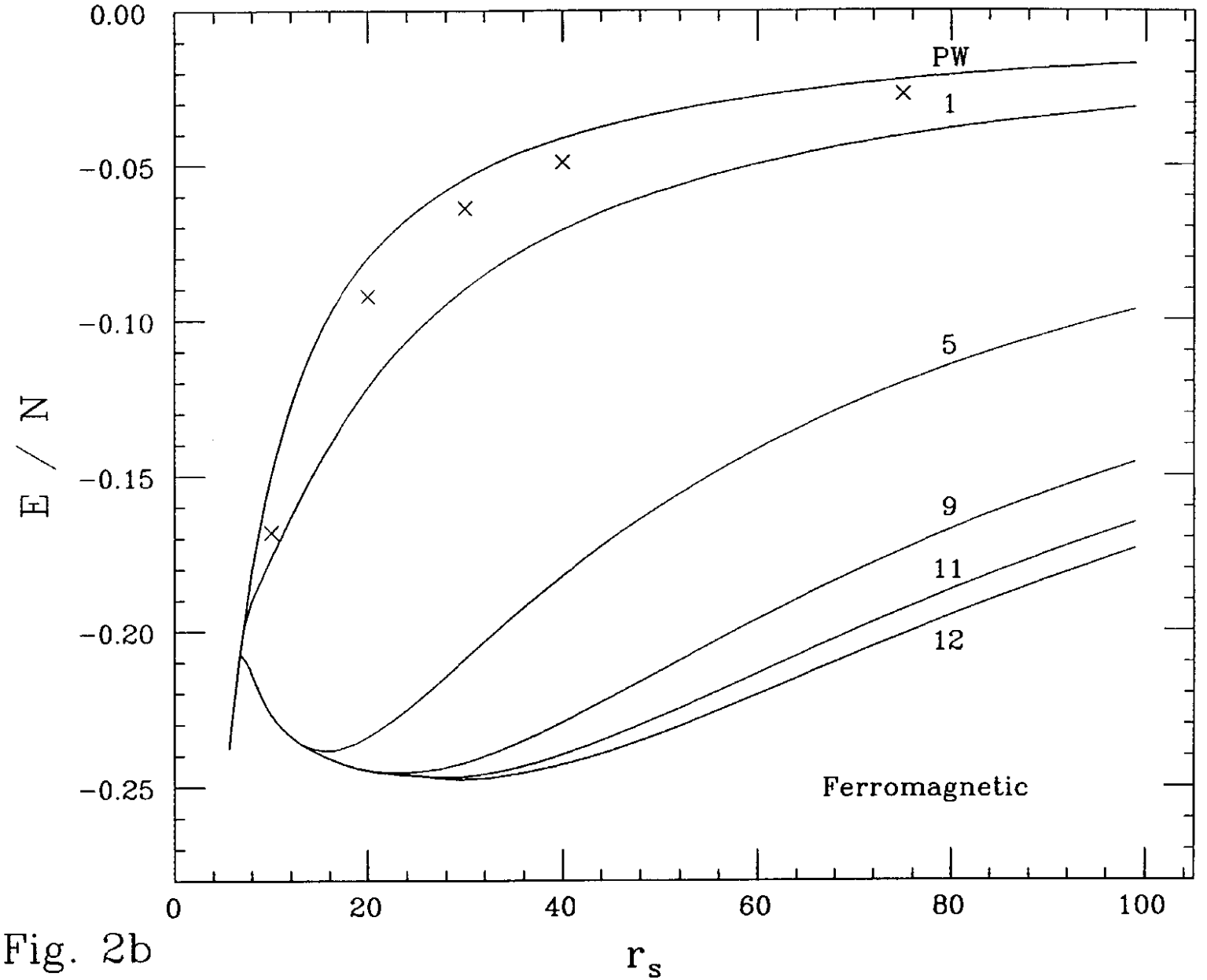
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Fig. 2b

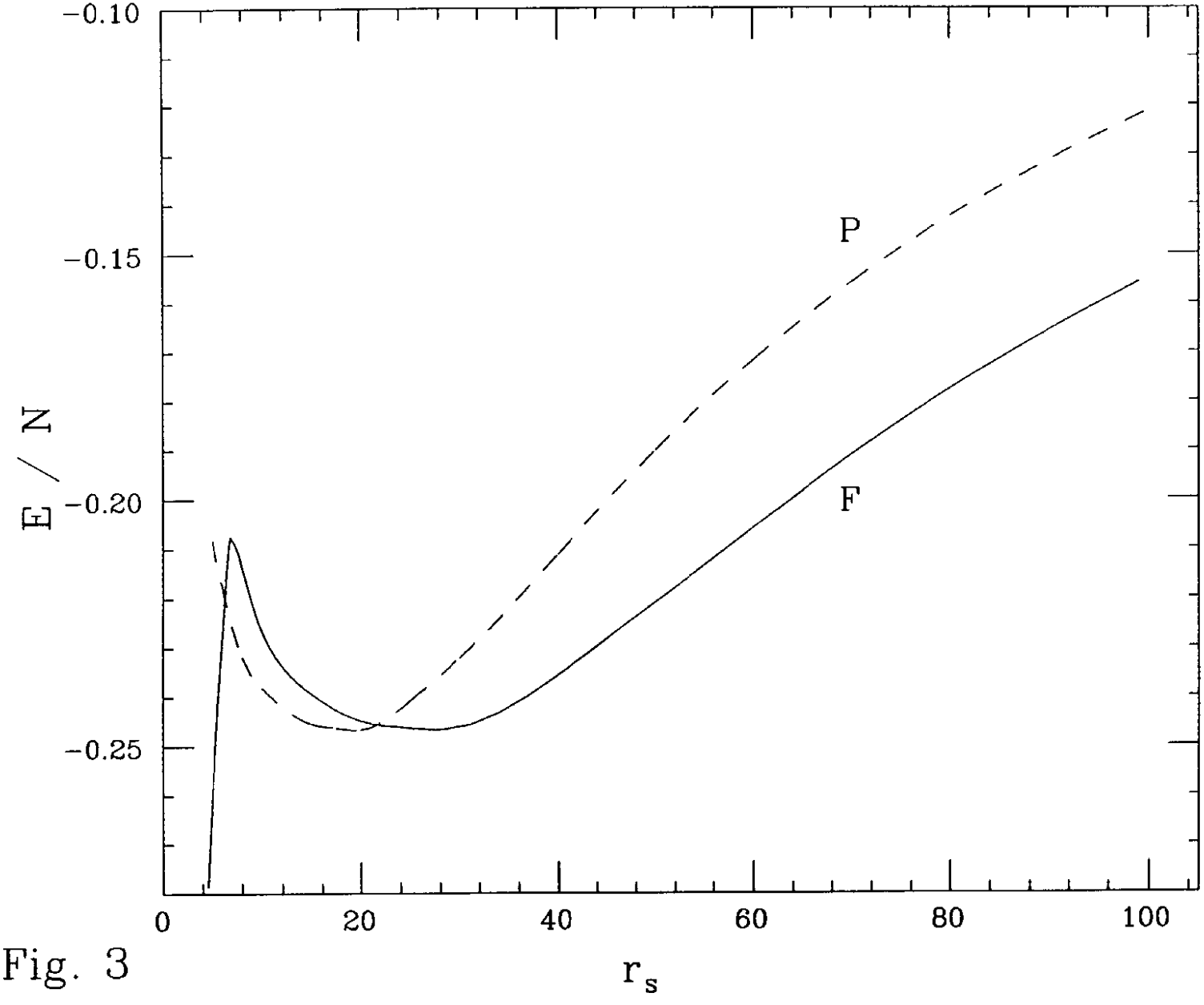

Fig. 3